chain nodes :
    1   2   3   4   5   6   7   8   9   10   17   18   19   26   27   28   35   40   41   42
ring nodes :
    11   12   13   14   15   16   20   21   22   23   24   25   29   30   31   32   33   34
chain bonds :
    1-2   2-3   3-4   3-41   4-5   5-35   6-7   6-35   7-8   7-9   9-10   10-13   16-17   17-18   17-19   19-21
    24-26   25-42   26-27   27-28   27-31   34-40
ring bonds :
    11-12   11-16   12-13   13-14   14-15   15-16   20-21   20-25   21-22   22-23   23-24   24-25   29-30
    29-34   30-31   31-32   32-33   33-34
exact/norm bonds :
    3-4   3-41   6-7   6-35   7-8   9-10   10-13   17-18   17-19   19-21   24-26   26-27   27-28   34-40
exact bonds :
    1-2   2-3   4-5   5-35   7-9   16-17   25-42   27-31
normalized bonds :
    11-12   11-16   12-13   13-14   14-15   15-16   20-21   20-25   21-22   22-23   23-24   24-25   29-30
    29-34   30-31   31-32   32-33   33-34

Match level :
    1:CLASS   2:CLASS   3:CLASS   4:CLASS   5:CLASS   6:CLASS   7:CLASS   8:CLASS   9:CLASS   10:CLASS
    11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:CLASS   18:CLASS   19:CLASS   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:CLASS   27:CLASS   28:CLASS   29:Atom   30:Atom
    31:Atom   32:Atom   33:Atom   34:Atom   35:CLASS   40:CLASS   41:CLASS   42:CLASS